mathematics

Article

Eccentricity-Based Topological Indices of a Cyclic Octahedron Structure

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Received: 10 July 2018; Accepted: 9 August 2018; Published: 17 August 2018

Abstract: In this article, we study the chemical graph of a cyclic octahedron structure of dimension n and compute the eccentric connectivity polynomial, the eccentric connectivity index, the total eccentricity, the average eccentricity, the first Zagreb index, the second Zagreb index, the third Zagreb index, the atom bond connectivity index and the geometric arithmetic index of the cyclic octahedron structure. Furthermore, we give the analytically closed formulas of these indices which are helpful for studying the underlying topologies.

Keywords: molecular graph; eccentric connectivity polynomial; eccentric connectivity index; total eccentricity; average eccentricity; first Zagreb index; second Zagreb index; third Zagreb index; atom bond connectivity index; geometric arithmetic index; cyclic Octahedron structure

JEL Classification: 05C12; 05C90

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1. Introduction

Graph theory has advanced greatly in the field of mathematical chemistry. Chemical graph theory has become very popular among researchers because of its wide application in mathematical chemistry. The molecular topological descriptors are the numerical invariants of a molecular graph and are very useful for predicting their bioactivity. A great variety of such indices have been studied and used in theoretical chemistry, by pharmaceutical researchers, in drugs, and in other different fields. There is considerable usage of graph theory in chemistry. Chemical graph theory is the topology branch of mathematical chemistry which applies graph theory to the mathematical modeling of chemical occurrence. A lot of research has been done in this area in the last few decades. This theory has a major role in the field of chemical sciences.

In reference [1,2], W. Gao et al. computed the electron energy of molecular structures through the forgotten topological index. Also, they computed the generalized atom bond connectivity index of several chemical molecular graphs. In reference [3–5], the authors studied topological indices of networks and nanotubes. The topological index of aztec diamonds was discussed in reference [6] by M. Imran et al. Some degree-based and eccentricity-based topological indices of oxide networks and tetra sheets were described in reference [7–9] by A. Q. Baig et al., respectively.

Recently the eccentric atom bond connectivity index of linear polycene parallelogram benzenoid was introduced by reference [10]. Sierpinski graphs constitute an extensively studied family of graphs of fractal nature and have been applied in topology, the mathematics of the Tower of Hanoi, computer science, and elsewhere [11]. The Sierpinski graphs were introduced in reference [12] by Klavzar and Milutinovic. The average eccentricity and standard deviation for all Sierpiński graphs (S_p^n) was established by reference [13]. The extremal properties of the average eccentricity as well as the conjectures and autographics were obtained by reference [14], in which the AutoGraphiX(AGX) computer system was developed by the GERAD group from Montreal [15–17]. AGX is an interactive software designed to help find conjectures in graph theory. The bounds on the mean eccentricity of graph and also the change in mean eccentricity when a graph is replaced by a subgraph was established by reference [18]. For trees with a fixed diameter, fixed matching number and fixed number of pendent vertices, the lower and upper bounds of average eccentricity were found by reference [19].

An undirected graph is a pair ($G = (V, E)$), where V is the set of vertices, and $E \subseteq \binom{V}{2}$ is a set of edges. In molecular graph theory, the vertices represent atoms, and the edges represent bonds between the atoms.

If $u, v \in V$, then the distance ($d(u, v)$) between u and v is defined as the length of any shortest path in G connecting u and v. We denote d_v as the number of edges incident to vertex v in G. The eccentricity of u is the distance of vertex u from the farthest vertex in G. In mathematical form, this is shown as $\varepsilon(u) = \max\{d(u, v) | \forall\ v \in V\}$. Table 1 describes the eccentricity-based indices and polynomials which have been introduced over the years.

Table 1. Eccentric-based indices.

S.No.	Introduced by	Index Name	Notation	Formula
1	V. Sharma et al. [20]	Eccentric connectivity index	$\xi(G)$	$\sum_{v\in V} d_v\varepsilon(v)$
2	M. Alaeiyan et al. [21,22]	Eccentric connectivity polynomial	$ECP(G,x)$	$\sum_{v\in V} d_v x^{\varepsilon(v)}$
3	Farooq et al. [23]	Total eccentricity index	$\zeta(G)$	$\sum_{v\in V} \varepsilon(v)$
4	F. Bukley et al. [24]	Average eccentricity	$avec(G)$	$\frac{1}{n}\sum_{v\in V} \varepsilon(v)$
5	D. Vukičević et al. Ghorbani et al. [25,26]	First Zagreb eccentric index Second Zagreb eccentric index third Zagreb eccentric index	$M_1^*(G)$ $M_1^{**}(G)$ $M_2^*(G)$	$\sum_{uv\in E} [\varepsilon(u)+\varepsilon(v)]$ $\sum_{v\in V} [\varepsilon(v)]^2$ $\sum_{uv\in E} \varepsilon(u)\varepsilon(v)$
6	M. Ghorbani et al. [27]	Geometric-arithmetic index	$GA_4(G)$	$\sum_{uv\epsilon E(G)} \frac{2\sqrt{\varepsilon(u)\cdot\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$
7	Farahani [28]	ABC eccentric index	$ABC_5(G)$	$\sum_{uv\in E(G)} \sqrt{\frac{\varepsilon(v)+\varepsilon(u)-2}{\varepsilon(v)\cdot\varepsilon(u)}}$

The aim of this paper is to compute and compare the above described eccentric-based topological indices for a cyclic octahedron structure of dimension n.

2. Main Results and Discussion

In this section, we discuss the cyclic octahedron structure and give closed formulae of certain topological indices for this network. Here, we find the analytically closed results of the eccentric connectivity polynomial, the eccentric connectivity index, the total eccentricity index, the average eccentricity index, and the eccentricity-based geometric-arithmetic and atom bond connectivity indices for the cyclic octahedron structure.

An octahedron graph, as shown in Figure 1, is a polyhedral graph corresponding to the skeleton of the octahedron, one of the five Platonic solids. This Platonic graph consists of six vertices and 12 edges. The analogs of this structure play vital roles in the field of reticular chemistry, which deals with the synthesis and properties of metal-organic frameworks [11,29].

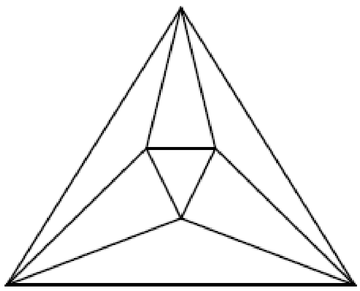

Figure 1. Structure of an octahedron.

The different types of octahedral structures arise from the ways that these octahedra can be connected. The cyclic octahedral structure of dimension n is denoted by CYO_n, and it is obtained by arranging n octahedra in cyclic order, as shown in Figure 2. For $n \geq 3$, CYO_n consists of $5n$ vertices and $12n$ edges. To compute the said indices and polynomials, we partitioned the vertices and edges of CYO_n in certain ways in Tables 2–7. To understand the tables and the partitions that they describe, we give detailed captions of each table. We computed the exact formulas for the above mentioned topological indices of the cyclic octahedral structure as follows.

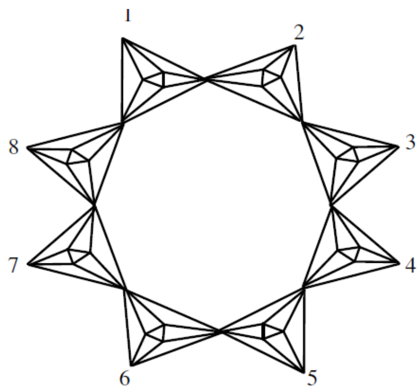

Figure 2. Cyclic octahedral structure (CYO_8).

Table 2. Vertex partition of the cyclic octahedron structure for (n-levels) where n is odd based on the degree and eccentricity of each vertex with the existence of their frequencies.

d_u	$\varepsilon(u)$	Frequency	Range of n
4	$\frac{n+3}{2}$	$4n$	$n \geq 3$
8	$\frac{n+1}{2}$	n	$n \geq 3$

Table 3. Vertex partition of the cyclic octahedron structure for (n-levels) where n is even based on the degree and eccentricity of each vertex with the existence of their frequencies.

d_u	$\varepsilon(u)$	Frequency	Range of n
4	$\frac{n+2}{2}$	$2n$	$n \geq 4$
4	$\frac{n+4}{2}$	$2n$	$n \geq 4$
8	$\frac{n+2}{2}$	n	$n \geq 4$

Table 4. Vertex partition of the cyclic octahedron structure for (n-levels) where n is odd based on the eccentricity of each vertex with the existence of their frequencies.

$\varepsilon(u)$	Frequency	Range of n
$\frac{n+1}{2}$	n	$n \geq 3$
$\frac{n+3}{2}$	$4n$	$n \geq 3$

Table 5. Vertex partition of the cyclic octahedron structure for (n-levels) where n is even based on the eccentricity of each vertex with existence of their frequencies.

$\varepsilon(u)$	Frequency	Range of n
$\frac{n+2}{2}$	$3n$	$n \geq 4$
$\frac{n+4}{2}$	$2n$	$n \geq 4$

Table 6. Edge partition of the cyclic octahedron structure for (n-levels) where n is odd based on the eccentricity of end vertices with the existence of their frequencies.

$(\varepsilon(u), \varepsilon(v))$	Frequency	Range of n
$(\frac{n+1}{2}, \frac{n+1}{2})$	n	$n \geq 3$
$(\frac{n+1}{2}, \frac{n+3}{2})$	$6n$	$n \geq 3$
$(\frac{n+3}{2}, \frac{n+3}{2})$	$5n$	$n \geq 3$

Table 7. Edge partition of the cyclic octahedron structure for (n-levels) where n is even, based on the eccentricity of end vertices with the existence of their frequencies.

$(\varepsilon(u), \varepsilon(v))$	Frequency	Range of n
$(\frac{n+2}{2}, \frac{n+2}{2})$	$5n$	$n \geq 4$
$(\frac{n+2}{2}, \frac{n+4}{2})$	$6n$	$n \geq 4$
$(\frac{n+4}{2}, \frac{n+4}{2})$	n	$n \geq 4$

2.1. Eccentric Connectivity Polynomial

Then, using the following theorems, we computed the eccentric polynomial of the cyclic octahedron structure ($ECP(CYO_n, x)$).

Theorem 1. *Let CYO_n, for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the eccentric polynomial of CYO_n is*

$$ECP(CYO_n, x) = 8n\{2x+1\}x^{\frac{n+1}{2}}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the eccentric polynomial is

$$ECP(G, x) = \sum_{v \in V} d_v x^{\varepsilon(v)}.$$

Using the vertex partition from Table 1, we obtained the following computations:

$$ECP(CYO_n, x) = 4 \cdot 4n \cdot (x)^{\frac{n+3}{2}} + 8 \cdot n \cdot (x)^{\frac{n+1}{2}},$$

$$ECP(CYO_n, x) = 16n \cdot (x)^{\frac{n+3}{2}} + 8n \cdot (x)^{\frac{n+1}{2}},$$

$$ECP(CYO_n, x) = 8n\{2x+1\}x^{\frac{n+1}{2}}.$$

□

Theorem 2. *Let CYO_n, for all $n \geq 4$ where n is even, be the cyclic octahedron structure. Then, the eccentric polynomial of CYO_n is*

$$ECP(CYO_n, x) = 8n\{x+2\}x^{\frac{n+2}{2}}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the eccentric polynomial is

$$ECP(G, x) = \sum_{v \in V} d_v x^{\varepsilon(v)}.$$

Using the vertex partition from Table 2, we obtained the following computations:

$$ECP(CYO_n, x) = 8 \cdot n \cdot (x)^{\frac{n+2}{2}} + 8 \cdot n \cdot (x)^{\frac{n+4}{2}} + 8 \cdot n \cdot (x)^{\frac{n+2}{2}},$$

$$ECP(CYO_n, x) = 8n \cdot (x)^{\frac{n+4}{2}} + 16n \cdot (x)^{\frac{n+2}{2}},$$

$$ECP(CYO_n, x) = 8n\{x+2\}x^{\frac{n+2}{2}}.$$

□

2.2. Eccentric Connectivity Index

Then, using the following theorems, we computed the eccentric connectivity index of the cyclic octahedron structure ($\xi(CYO_n)$).

Theorem 3. *Let CYO_n, for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the eccentric connectivity index of CYO_n is*

$$\xi(CYO_n) = 4n\{3n+7\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the eccentric connectivity index is:

$$\xi(G) = \sum_{v \in V} d_v \varepsilon(v).$$

Using the vertex partition from Table 1, we obtained the following computations:

$$\xi(CYO_n) = 4 \cdot 4n \cdot \left(\frac{n+3}{2}\right) + 8 \cdot n \cdot \left(\frac{n+1}{2}\right),$$

$$\xi(CYO_n) = 8n \cdot (n+3) + 4n \cdot (n+1),$$

$$\xi(CYO_n) = 4n\{3n+7\}.$$

□

Theorem 4. *Let CYO_n, for all $n \geq 4$, where n is even, be the cyclic octahedron structure. Then, the eccentric connectivity index of CYO_n is*

$$\xi(CYO_n) = 4n\{3n+8\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the eccentric connectivity index is

$$\xi(G) = \sum_{v \in V} d_v \varepsilon(v).$$

Using the vertex partition from Table 2, we obtained the following computations:

$$\xi(CYO_n) = 4 \cdot (2n) \cdot \left(\frac{n+2}{2}\right) + 4 \cdot (2n) \cdot \left(\frac{n+4}{2}\right) + 8 \cdot n \cdot \left(\frac{n+2}{2}\right),$$

$$\xi(CYO_n) = 4n \cdot (n+4) + 8n \cdot (n+2),$$

$$\xi(CYO_n) = 4n\{3n+8\}.$$

□

2.3. Total Eccentricity Index

Then, using the following theorems, we computed the total eccentricity index of the cyclic octahedron structure ($\zeta(CYO_n)$).

Theorem 5. *Let CYO_n, for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the total eccentricity index (ζ) of CYO_n is*

$$\zeta(CYO_n) = \frac{n}{2}\{5n+13\}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the total eccentricity index is

$$\zeta(G) = \sum_{v \in V(G)} \varepsilon(v).$$

Using the vertex partitioned from Table 3, we obtained the following computations:

$$\zeta(CYO_n) = n \cdot \left(\frac{n+1}{2}\right) + 4n \cdot \left(\frac{n+3}{2}\right),$$

$$\zeta(CYO_n) = \frac{n}{2}\{n+1+4n+12\},$$

$$\zeta(CYO_n) = \frac{n}{2}\{5n+13\}.$$

□

Theorem 6. *Let CYO_n, for all $n \geq 4$, where n is even, be the cyclic octahedron structure, then the total eccentricity index (ζ) of CYO_n is*

$$\zeta(CYO_n) = \frac{n}{2}\{5n+14\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the total eccentricity index is

$$\zeta(G) = \sum_{v \in V(G)} \varepsilon(v).$$

Using the vertex partitioned from Table 4, we obtained the following computations

$$\zeta(CYO_n) = 3n \cdot \left(\frac{n+2}{2}\right) + 2n \cdot \left(\frac{n+4}{2}\right),$$

$$\zeta(CYO_n) = \frac{n}{2}\{3n + 6 + 2n + 8\},$$

$$\zeta(CYO_n) = \frac{n}{2}\{5n + 14\}.$$

□

2.4. Average Eccentricity Index

In this section, we describe how the average eccentricity index of the cyclic octahedron structure ($avec(CYO_n)$) was determined.

Theorem 7. *Let CYO_n, for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the average eccentricity index ($avec(CYO_n)$) is*

$$avec(CYO_n) = \frac{1}{10}\{5n + 13\}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the average eccentricity index is

$$avec(G) = \frac{1}{n}\sum \varepsilon_i.$$

Using the vertex partitioned from Table 3, we obtained the following computations:

$$avec(CYO_n) = \frac{1}{5n}\left\{n \cdot \left(\frac{n+1}{2}\right) + 4n \cdot \left(\frac{n+3}{2}\right)\right\},$$

$$avec(CYO_n) = \frac{n}{10n}\{n + 1 + 4n + 12\},$$

$$avec(CYO_n) = \frac{1}{10}\{5n + 13\}.$$

□

Theorem 8. *Let CYO_n, for all $n \geq 4$, where n is even, be the cyclic octahedron structure. Then, the average eccentricity index ($avec(CYO_n)$) is*

$$avec(CYO_n) = \frac{1}{10}\{5n + 14\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The formula of the average eccentricity index is

$$avec(G) = \frac{1}{n}\sum \varepsilon_i.$$

Using the vertex partitioned from Table 4, we obtained the following computations:

$$avec(CYO_n) = \frac{1}{5n}\left\{3n \cdot \left(\frac{n+2}{2}\right) + 2n \cdot \left(\frac{n+4}{2}\right)\right\},$$

$$avec(CYO_n) = \frac{n}{10n}\{3n+6+2n+8\},$$
$$avec(CYO_n) = \frac{1}{10}\{5n+14\}.$$

□

2.5. First Zagreb Eccentricity Index

In this section, we describe how we found the first Zagreb eccentricity index of the cyclic octahedron structure ($M_1^*(CYO_n)$).

Theorem 9. *Let CYO_n for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the first Zagreb eccentricity index $M_1^*(CYO_n)$ is*

$$M_1^*(CYO_n) = 4n\{3n+7\}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the first Zagreb eccentricity index is

$$M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)].$$

By using the values from Table 5, we obtained

$$M_1^*(CYO_n) = n\left(\frac{n+1}{2} + \frac{n+1}{2}\right) + 6n\left(\frac{n+1}{2} + \frac{n+3}{2}\right) + 5n\left(\frac{n+3}{2} + \frac{n+3}{2}\right),$$
$$M_1^*(CYO_n) = n(n+1) + 6n(n+2) + 5n(n+3),$$
$$M_1^*(CYO_n) = 4n\{3n+7\}.$$

□

Theorem 10. *Let CYO_n for all $n \geq 4$, where n is even, be the cyclic octahedron structure. Then, the first Zagreb eccentricity index ($M_1^*(CYO_n)$) is*

$$M_1^*(CYO_n) = 4n\{3n+8\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the first Zagreb eccentricity index is

$$M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)].$$

By using the values from Table 6, we obtained

$$M_1^*(CYO_n) = 5n\left(\frac{n+2}{2} + \frac{n+2}{2}\right) + 6n\left(\frac{n+2}{2} + \frac{n+4}{2}\right) + n\left(\frac{n+4}{2} + \frac{n+4}{2}\right),$$
$$M_1^*(CYO_n) = 5n(n+2) + 6n(n+3) + n(n+4),$$
$$M_1^*(CYO_n) = 4n\{3n+8\}.$$

□

2.6. Second Zagreb Eccentricity Index

In this section, we describe how we found the second Zagreb eccentricity index of the cyclic octahedron structure ($M_1^{**}(CYO_n)$).

Theorem 11. *Let CYO_n for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the second Zagreb eccentricity index ($M_1^{**}(CYO_n)$) is*

$$M_1^{**}(CYO_n) = \frac{n}{4}\{5n^2 + 26n + 37\}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the second Zagreb eccentricity index is

$$M_1^{**}(G) = \sum_{v \in V(G)} [\varepsilon(v)]^2.$$

By using the values from Table 3, we obtained

$$M_1^{**}(CYO_n) = n\left(\frac{n+1}{2}\right)^2 + 4n\left(\frac{n+3}{2}\right)^2,$$

$$M_1^{**}(CYO_n) = \frac{n}{4}(n^2 + 2n + 1 + 4n^2 + 24n + 36),$$

$$M_1^{**}(CYO_n) = \frac{n}{4}\{5n^2 + 26n + 37\}.$$

□

Theorem 12. *Let CYO_n for all $n \geq 4$, where n is even, be the cyclic octahedron structure. Then, the second Zagreb eccentricity index ($M_1^{**}(CYO_n)$) is*

$$M_1^{**}(CYO_n) = \frac{n}{4}\{5n^2 + 28n + 44\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the second Zagreb eccentricity index is

$$M_1^{**}(G) = \sum_{v \in V(G)} [\varepsilon(v)]^2.$$

By using the values from Table 4, we obtained

$$M_1^{**}(CYO_n) = 3n\left(\frac{n+2}{2}\right)^2 + 2n\left(\frac{n+4}{2}\right)^2,$$

$$M_1^{**}(CYO_n) = \frac{n}{4}(3n^2 + 12n + 12 + 2n^2 + 16n + 32) = \frac{n}{4}\{5n^2 + 28n + 44\}.$$

□

2.7. Third Zagreb Eccentricity Index

In this section we describe how we found the third Zagreb eccentricity index of the cyclic octahedron structure ($M_2^{*}(CYO_n)$).

Theorem 13. *Let CYO_n for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the third Zagreb eccentricity index ($M_2^*(CYO_n)$) is*

$$M_2^*(CYO_n) = n\{3n^2 + 14n + 16\}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the third Zagreb eccentricity index is

$$M_2^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) \cdot \varepsilon(v)].$$

By using the values from Table 5, we obtained

$$M_2^*(CYO_n) = n\left(\frac{n+1}{2} \cdot \frac{n+1}{2}\right) + 6n\left(\frac{n+1}{2} \cdot \frac{n+3}{2}\right) + 5n\left(\frac{n+3}{2} \cdot \frac{n+3}{2}\right),$$

$$M_2^*(CYO_n) = n\left(\frac{n+1}{2}\right)^2 + 6n\left(\frac{n^2+4n+3}{4}\right) + 5n\left(\frac{n+3}{2}\right)^2,$$

$$M_2^*(CYO_n) = n\{3n^2 + 14n + 16\}.$$

□

Theorem 14. *Let CYO_n for all $n \geq 4$, where n is even, be the cyclic octahedron structure. Then, the third Zagreb eccentricity index $M_2^*(CYO_n)$ is*

$$M_2^*(CYO_n) = n\{3n^2 + 16n + 21\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure contains $5n$ vertices and $12n$ edges.

The general formula of the third Zagreb eccentricity index is

$$M_2^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) \cdot \varepsilon(v)].$$

By using the values from Table 6, we obtained

$$M_2^*(CYO_n) = 5n\left(\frac{n+2}{2} \cdot \frac{n+2}{2}\right) + 6n\left(\frac{n+2}{2} \cdot \frac{n+4}{2}\right) + n\left(\frac{n+4}{2} \cdot \frac{n+4}{2}\right),$$

$$M_2^*(CYO_n) = 5n\left(\frac{n+2}{2}\right)^2 + 6n\left(\frac{n^2+6n+8}{4}\right) + n\left(\frac{n+4}{2}\right)^2,$$

$$M_2^*(CYO_n) = n\{3n^2 + 16n + 21\}.$$

□

2.8. Geometric-Arithmetic Index

In this section, we describe how we found the eccentricity-based geometric-arithmetic index of the cyclic octahedron structure $GA_4(CYO_n)$.

Theorem 15. *Let CYO_n for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then the geometric-arithmetic index ($GA_4(CYO_n)$) is*

$$GA_4(CYO_n) = 6n\left\{1 + \frac{\sqrt{n^2+4n+3}}{n+2}\right\}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the eccentricity-based geometric-arithmetic index is

$$GA_4(G) = \sum_{uv\epsilon E(G)} \frac{2\sqrt{\varepsilon(u)\cdot\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}.$$

Using the edge partitioned from Table 5, we obtained the following computations:

$$GA_4(CYO_n) = n\left(\frac{2\sqrt{\frac{n+1}{2}\cdot\frac{n+1}{2}}}{\frac{n+1}{2}+\frac{n+1}{2}}\right) + 6n\left(\frac{2\sqrt{\frac{n+1}{2}\cdot\frac{n+3}{2}}}{\frac{n+1}{2}+\frac{n+3}{2}}\right) + 5n\left(\frac{2\sqrt{\frac{n+3}{2}\cdot\frac{n+3}{2}}}{\frac{n+3}{2}+\frac{n+3}{2}}\right),$$

$$GA_4(CYO_n) = n\left(\frac{2\sqrt{(\frac{n+1}{2})^2}}{n+1}\right) + 6n\left(\frac{\sqrt{n^2+4n+3}}{n+2}\right) + 5n\left(\frac{2\sqrt{(\frac{n+3}{2})^2}}{n+3}\right),$$

$$GA_4(CYO_n) = 6n\left\{1 + \frac{\sqrt{n^2+4n+3}}{n+2}\right\}.$$

□

Theorem 16. *Let CYO_n for all $n \geq 4$, where n is even, be the cyclic octahedron structure. Then the geometric-arithmetic index ($GA_4(CYO_n)$) is*

$$GA_4(CYO_n) = 6n\left\{1 + \frac{\sqrt{n^2+6n+8}}{n+3}\right\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the eccentricity-based geometric-arithmetic index is

$$GA_4(G) = \sum_{uv\epsilon E(G)} \frac{2\sqrt{\varepsilon(u)\cdot\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}.$$

Using the edge partitioned from Table 6, we obtained the following computations:

$$GA_4(CYO_n) = 5n\left(\frac{2\sqrt{\frac{n+2}{2}\cdot\frac{n+2}{2}}}{\frac{n+2}{2}+\frac{n+2}{2}}\right) + 6n\left(\frac{2\sqrt{\frac{n+2}{2}\cdot\frac{n+4}{2}}}{\frac{n+2}{2}+\frac{n+4}{2}}\right) + n\left(\frac{2\sqrt{\frac{n+4}{2}\cdot\frac{n+4}{2}}}{\frac{n+4}{2}+\frac{n+4}{2}}\right),$$

$$GA_4(CYO_n) = 5n\left(\frac{2\sqrt{(\frac{n+2}{2})^2}}{n+2}\right) + 6n\left(\frac{\sqrt{n^2+6n+8}}{n+3}\right) + n\left(\frac{2\sqrt{(\frac{n+4}{2})^2}}{n+4}\right),$$

$$GA_4(CYO_n) = 6n\left\{1 + \frac{\sqrt{n^2+6n+8}}{n+3}\right\}.$$

□

2.9. Atom Bond Connectivity Index

In this section, we desscribe how we found the eccentricity-based atom bond connectivity index of the cyclic octahedron structure ($ABC_5(CYO_n)$).

Theorem 17. *Let CYO_n for all $n \geq 3$, where n is odd, be the cyclic octahedron structure. Then, the atom bond connectivity index ($ABC_5(CYO_n)$) is*

$$ABC_5(CYO_n) = 2n\left\{\frac{\sqrt{n-1}}{n+1} + \frac{5\sqrt{n+1}}{n+3} + 6\sqrt{\frac{n}{n^2+4n+3}}\right\}.$$

Proof. Let CYO_n, where n is odd, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the eccentricity-based atom bond connectivity index is

$$ABC_5(G) = \sum_{uv\epsilon E(G)} \sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\cdot\varepsilon(v)}}.$$

Using the edge partitioned from Table 5, we obtained the following computations:

$$ABC_5(CYO_n) = n\sqrt{\frac{\frac{n+1}{2}+\frac{n+1}{2}-2}{\frac{n+1}{2}\cdot\frac{n+1}{2}}} + 6n\sqrt{\frac{\frac{n+1}{2}+\frac{n+3}{2}-2}{\frac{n+1}{2}\cdot\frac{n+3}{2}}} + 5n\sqrt{\frac{\frac{n+3}{2}+\frac{n+3}{2}-2}{\frac{n+3}{2}\cdot\frac{n+3}{2}}},$$

$$ABC_5(CYO_n) = n\sqrt{\frac{n+1-2}{(\frac{n+1}{2})^2}} + 12n\sqrt{\frac{n+2-2}{n^2+4n+3}} + 5n\sqrt{\frac{n+3-2}{(\frac{n+3}{2})^2}},$$

$$ABC_5(CYO_n) = 2n\left\{\frac{\sqrt{n-1}}{n+1} + \frac{5\sqrt{n+1}}{n+3} + 6\sqrt{\frac{n}{n^2+4n+3}}\right\}.$$

□

Theorem 18. *Let CYO_n for all $n \geq 4$, where n is even, be the cyclic octahedron structure. Then the atom bond connectivity index ($ABC_5(CYO_n)$) is*

$$ABC_5(CYO_n) = 2n\left\{\frac{5\sqrt{n}}{n+2} + \frac{\sqrt{n+2}}{n+4} + 6\sqrt{\frac{n+1}{n^2+6n+8}}\right\}.$$

Proof. Let CYO_n, where n is even, be the cyclic octahedron structure containing $5n$ vertices and $12n$ edges.

The general formula of the eccentricity-based atom bond connectivity index is

$$ABC_5(G) = \sum_{uv\epsilon E(G)} \sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\cdot\varepsilon(v)}}.$$

Using the edge partitioned from Table 6, we obtained the following computations:

$$ABC_5(CYO_n) = 5n\sqrt{\frac{\frac{n+2}{2}+\frac{n+2}{2}-2}{\frac{n+2}{2}\cdot\frac{n+2}{2}}} + 6n\sqrt{\frac{\frac{n+2}{2}+\frac{n+4}{2}-2}{\frac{n+2}{2}\cdot\frac{n+4}{2}}} + n\sqrt{\frac{\frac{n+4}{2}+\frac{n+4}{2}-2}{\frac{n+4}{2}\cdot\frac{n+4}{2}}},$$

$$ABC_5(CYO_n) = 5n\sqrt{\frac{n+2-2}{(\frac{n+2}{2})^2}} + 12n\sqrt{\frac{n+3-2}{n^2+6n+8}} + n\sqrt{\frac{n+4-2}{(\frac{n+4}{2})^2}},$$

$$ABC_5(CYO_n) = 2n\left\{\frac{5\sqrt{n}}{n+2} + \frac{\sqrt{n+2}}{n+4} + 6\sqrt{\frac{n+1}{n^2+6n+8}}\right\}.$$

□

3. Comparison

In this section, we present tabular and graphical comparisons of the above computed indices. Table 8 shows a comparison of the eccentric connectivity index, total eccentricity, average eccentricity, first Zagreb index, second Zagreb index, third Zagreb index, atom bond connectivity index, and geometric arithmetic index for small values of n. Figure 3 shows a graphical comparison of the indices.

Table 8. Comparison of $\xi(G)$, $\zeta(G)$, $avec(G)$, $M_1^*(G)$, $M_1^{**}(G)$, $M_2^*(G)$, $GA_4(G)$, and $ABC_5(G)$ of $G \cong CYO_n$.

n	$\xi(G)$	$\zeta(G)$	$avec(G)$	$M_1^*(G)$	$M_1^{**}(G)$	$M_2^*(G)$	$GA_4(G)$	$ABC_5(G)$
3	304	66	3.3	304	221	480	47.7	31.8
4	320	68	3.4	320	236	532	45.8	31.3
5	600	129	4.3	600	559.5	1248	71.8	43.7
6	624	132	4.4	624	588	1350	70	43.1
7	992	212	5.3	992	1130	2560	95.8	53.8
8	1024	216	5.4	1024	1176	2728	92.5	53.1
9	1480	315	6.3	1480	1992.5	4560	119.8	62.7
10	1520	320	6.4	1520	2060	4810	116.2	62.1

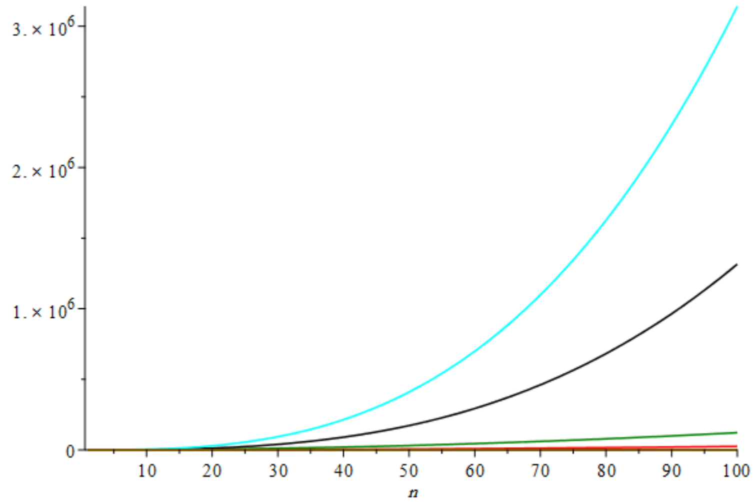

Figure 3. Graphical behavior of the eccentric indices of the cyclic octahedron structure with different colors: $\xi(G)$ is green, $\zeta(G)$ is red, $avec(G)$ is blue, $M_1^*(G) = \xi(G)$, $M_1^{**}(G)$ is black, $M_2^*(G)$ is cyan, $GA_4(G)$ is gold, and $ABC_5(G)$ is orange.

4. Conclusions

As depicted above in Figure 3 and Table 8, one can easily see the different aspects of behavior of the cyclic octahedron structure with respect to the eccentric-based indices.

Author Contributions: The contributions of author is as; The concept, editing and supervision of the article was given by Abdul Qudair Baig. All the computations, main editing of text and use of software were made by Muhammad Naeem. Data collection and correction was made by Manzoor Ahmed Zahid. The investigation, writing first draft and methodology of the proof was done by Muhammad Razwan Azhar.

Funding: This research received no external funding.

Conflicts of Interest: The authors declare no conflict of interest.

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